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STRUCTURE FILE UPDATES: 3 AUG 2008 HIGHEST RN 1038266-69-1 DICTIONARY FILE UPDATES: 3 AUG 2008 HIGHEST RN 1038266-69-1

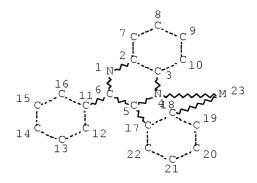
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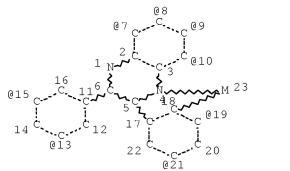
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89 ANSWERS

=> d 17 L7 HAS NO ANSWERS L7 STR



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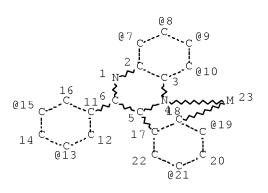
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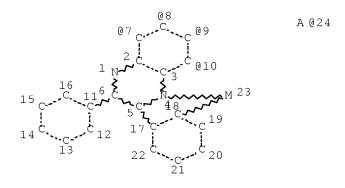
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DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES: RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 26

STEREO ATTRIBUTES: NONE

=> d que stat 19 L9 STR



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NSPEC IS RC AT 24
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
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NUMBER OF NODES IS 24

STEREO ATTRIBUTES: NONE

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(FILE 'HOME' ENTERED AT 16:15:14 ON 04 AUG 2008)

FILE 'HCAPLUS' ENTERED AT 16:15:25 ON 04 AUG 2008 E US20070241667/PN

L1 1 S E3 SEL RN

FILE 'REGISTRY' ENTERED AT 16:15:49 ON 04 AUG 2008 L2 26 S E1-26

FILE 'LREGISTRY' ENTERED AT 16:17:12 ON 04 AUG 2008 L3

FILE 'REGISTRY' ENTERED AT 16:20:48 ON 04 AUG 2008

L4 6 S L3 L5 89 S L3 FUL L6 8 S L2 AND L5 SAV L5 YAM703/A FILE 'LREGISTRY' ENTERED AT 16:22:32 ON 04 AUG 2008 STR L3

FILE 'REGISTRY' ENTERED AT 16:29:42 ON 04 AUG 2008

L8 0 S L7 SSS SAM SUB=L5

L9 STR L7

L10 0 S L9 SSS SAM SUB=L5

FILE 'HCAPLUS' ENTERED AT 16:31:06 ON 04 AUG 2008

L11 41 S L5

L12 14 S L11 AND (PY<=2004 OR PRY<=2004 OR AY<=2004)

L13 27 S L11 NOT L12

=> fil hcap

L7

FILE 'HCAPLUS' ENTERED AT 16:34:19 ON 04 AUG 2008
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FILE COVERS 1907 - 4 Aug 2008 VOL 149 ISS 6 FILE LAST UPDATED: 3 Aug 2008 (20080803/ED)

HCAplus now includes complete International Patent Classification (IPC) reclassification data for the second quarter of 2008.

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This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d 112 ibib abs hitstr hitind 1-14

L12 ANSWER 1 OF 14 HCAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 2006:991036 HCAPLUS Full-text

DOCUMENT NUMBER: 145:497301

TITLE: Organic light emitting diode containing a novel

Ir complex as a red color phosphorescent emitter

INVENTOR(S): Chi, Yun; Chou, Pi-Tai; Kavitha, Jakka; Song,

Yi-Hwa; Chen, Hsing-Yi

PATENT ASSIGNEE(S): National Tsing Hua University, Taiwan

SOURCE: Taiwan., 4pp.

CODEN: TWXXA5

DOCUMENT TYPE: Patent LANGUAGE: Chinese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
 TW 231157	В	20050411	TW 2004-93117691	200406
			<	18
PRIORITY APPLN. INFO.:			TW 2004-93117691	200406 18

This invention provides a systematic method for syntheses of new electroluminescent iridium metal complexes by introducing chelating ligands such as quinoxaline, quinazoline, and pyrimidine. For utilization of quinoxaline, quinazoline or pyrimidine ligands, the strategy of substituting the carbon atom with the highly electroneg. nitrogen atom or extending the delocalization of pi electrons on the chelating aromatic chromophores can not only enhance the rigidity of the ligands and suppress the non-radiative decay, but also alter the electronic structures of the coordinating ligands. As a result, the energy gaps between the HOMO and LUMO orbitals, i.e. the energy gaps of IL (pipi*) or MLCT transitions are significantly reduced, shifting the emission wavelengths to the region of saturated red color. These phosphorescent complexes can be used as the emitting or emitter dopant materials to fabricate the high efficiency OLEDs for various types of future,

flat panel display applications.

IT 848889-89-4 848889-92-9 848889-94-1
848889-96-3

RL: DEV (Device component use); TEM (Technical or engineered material use); USES (Uses)

(organic light emitting diode containing novel Ir complex as red color phosphorescent emitter)

RN 848889-89-4 HCAPLUS

CN Iridium, bis[2-(3-phenyl-2-quinoxalinyl- κ N1)phenyl- κ C][2-[5-(trifluoromethyl)-1H-pyrazol-3-yl- κ N2]pyridinato- κ N]-, (OC-6-14)- (CA INDEX NAME)

RN 848889-92-9 HCAPLUS

CN Iridium, bis[5-fluoro-2-[3-(4-fluorophenyl)-2-quinoxalinyl-

 κ N1]phenyl- κ C][2-[5-(trifluoromethyl)-1H-pyrazol-3-yl- κ N2]pyridinato- κ N]-, (OC-6-14)- (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 848889-94-1 HCAPLUS

CN Iridium, bis[5-fluoro-2-[3-(4-fluoropheny1)-2-quinoxaliny1- κ N1]pheny1- κ C][2-[5-(trifluoromethy1)-1H-1,2,4-triazol-3- y1- κ N2]pyridinato- κ N]-, (OC-6-14)- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

RN 848889-96-3 HCAPLUS

CN Iridium, $[2-[3-(1,1-dimethylethyl)-1H-pyrazol-5-yl-\kappa N1]$ pyridinato- $\kappa N]$ bis $[5-fluoro-2-[3-(4-fluorophenyl)-2-quinoxalinyl-<math>\kappa N1]$ phenyl- $\kappa C]$ -, (OC-6-14)- (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

IC ICM H05B033-14 ICS C09K011-00

CC 73-11 (Optical, Electron, and Mass Spectroscopy and Other Related Properties)

IT 84889-89-4 848889-92-9 848889-94-1 848889-96-3 866941-02-8 866941-03-9

914771-93-0

RL: DEV (Device component use); TEM (Technical or engineered material use); USES (Uses)

(organic light emitting diode containing novel Ir complex as red color phosphorescent emitter)

866941-05-1

L12 ANSWER 2 OF 14 HCAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 2006:579425 HCAPLUS $\underline{\text{Full-text}}$

DOCUMENT NUMBER: 145:249355

TITLE: Organometallic complexes as electroluminescent

devices and light-emitting components

INVENTOR(S): Inoue, Eiko; Shimogaki, Tomoko; Seo, Tetsuji
PATENT ASSIGNEE(S): Semiconductor Energy Laboratory Co., Ltd., Japan
SOURCE: Faming Zhuanli Shenqing Gongkai Shuomingshu, 55

pp.

CODEN: CNXXEV

DOCUMENT TYPE: Patent LANGUAGE: Chinese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
 CN 1781912	А	20060607	CN 2005-10128999	200512 05
US 20060159955	A1	20060720	< US 2005-274327	200511 16
JP 2006182775	А	20060713	< JP 2005-348632	200512 02

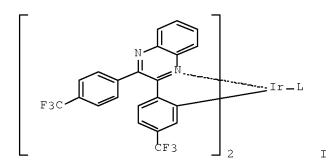
PRIORITY APPLN. INFO.:

<--JP 2004-352077

200412

OTHER SOURCE(S): MARPAT 145:249355

GΙ



AB This invention relates to an organometallic complex as shown in formula I, where L is single anion ligand containing β -diketone structure, single anion bidentate chelate complex containing carboxy, or single anion bidentate chelating ligands. This invention also relates to electroluminescent devices comprises the mentioned organometallic complexes, a light-emitting component layers, light-emitting substance and sensitizer of fluorescent compound IT 906369-47-9P 906369-49-1P

RL: DEV (Device component use); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)

(preparation of organoiridium complexes as electroluminescent device and phosphorescent light emitting component)

RN 906369-47-9 HCAPLUS

CN Iridium, $(2,4-pentanedionato-\kappa02,\kappa04)$ bis [5- $(trifluoromethyl)-2-[3-[4-(trifluoromethyl)phenyl]-2-quinoxalinyl-<math>\kappa$ N1]phenyl- κ C]- (CA INDEX NAME)

PAGE 1-A

RN 906369-49-1 HCAPLUS

CN Iridium, (2-pyridinecarboxylato- κ N1, κ O2)bis[5- (trifluoromethyl)-2-[3-[4-(trifluoromethyl)phenyl]-2-quinoxalinyl- κ N1]phenyl- κ C]- (9CI) (CA INDEX NAME)

IT 906369-48-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(reactant for preparation of organoiridium complexes as electroluminescent device and phosphorescent light emitting component)

RN 906369-48-0 HCAPLUS

CN Iridium, di- μ -chlorotetrakis[5-(trifluoromethyl)-2-[3-[4-(trifluoromethyl)phenyl]-2-quinoxalinyl- κ N1]phenyl- κ C]di-(9CI) (CA INDEX NAME)

PAGE 1-A

CC 29-13 (Organometallic and Organometalloidal Compounds)
 Section cross-reference(s): 73

IT 906369-47-9P 906369-49-1P
 RL: DEV (Device component use); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)

(preparation of organoiridium complexes as electroluminescent device and phosphorescent light emitting component)

IT 73790-20-2P 906369-46-8P 906369-48-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(reactant for preparation of organoiridium complexes as electroluminescent device and phosphorescent light emitting component)

L12 ANSWER 3 OF 14 HCAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 2006:578149 HCAPLUS Full-text

DOCUMENT NUMBER: 145:46196

TITLE: Organometallic complex, and light-emitting

element and light-emitting device using the same

DATE

INVENTOR(S): Inoue, Hideko; Shitagaki, Satoko; Seo, Satoshi
PATENT ASSIGNEE(S): Semiconductor Energy Laboratory Co., Ltd., Japan

PATENT NO. KIND DATE APPLICATION NO.

SOURCE: PCT Int. Appl., 84 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

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WO 2006	- 062144		A1		2006	0615	Ţ	WO 2	005-	JP22	507		2	00512 1
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	RO, RU, TZ, UA,	SC, UG,	SD, US,	SE, UZ,	SG, VC,	SK, VN,	SL, YU,	SM, ZA,	SY, ZM,	TJ, ZW	TM,	TN,	TR,	TT,
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US 2008	0113216		A1		2008	0515	1	US 2	007-	7924:	24		2	00706 6
RITY APP	LN. INFO.	:					ı	JP 2	< 004-3	3535	87	i	A 2 0	00412 7
							Ţ	wo 2	> 500	JP22	507	Ţ	W 2 0	00512 1

OTHER SOURCE(S): CASREACT 145:46196; MARPAT 145:46196

AB It is an object of the present invention to provide a substance capable of emitting phosphorescence. In addition, it is an object of the present invention to provide a light-emitting element that is excellent in chromaticity. One aspect of the present invention is preparation of organometallic complex I (R1-R4 = H, halo, acyl, alkyl, alkoxyl, aryl, cyano, heterocyclic; R5-R13 = H, acyl, alkyl, alkoxyl, aryl, heterocyclic, electron-withdrawing group). Thus, reaction of 2,3-bis(4-fluorophenyl)quinoxaline (preparation given) with K2[PtC14] in refluxing 2-ethoxyethanol/H2O followed by treatment with acetylacetone gave title compound, (acetylacetonato)[2,3-bis(4-fluorophenyl)quinoxalinato]platinum(II). An organometallic complex having such a structure can emit phosphorescence with higher emission intensity.

IT 889869-73-2P 889869-74-3P

RL: DEV (Device component use); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)

(preparation of cyclopatinated fluorophenyl quinoxaline organometallic complex and their use as light-emitting element and light-emitting device)

RN 889869-73-2 HCAPLUS

CN Platinum, [5-fluoro-2-[3-(4-fluoropheny1)-2-quinoxalinyl- κ N1]phenyl- κ C](2,4-pentanedionato- κ O, κ O')-, (SP-4-3)- (9CI) (CA INDEX NAME)

RN 889869-74-3 HCAPLUS

CN Platinum, $[2-[3-(3,5-difluorophenyl)-2-quinoxalinyl-\kappa N1]-4,6-difluorophenyl-\kappa C](2,4-pentanedionato-\kappa O,\kappa O')-, (SP-4-3)- (9CI) (CA INDEX NAME)$

IT 889869-72-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of cyclopatinated fluorophenyl quinoxaline organometallic complex and their use as light-emitting element and light-emitting device)

RN 889869-72-1 HCAPLUS

CN Platinum, $di-\mu$ -chlorobis[5-fluoro-2-[3-(4-fluorophenyl)-2-quinoxalinyl- κ N1]phenyl- κ C]di- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 2-A



CC 29-13 (Organometallic and Organometalloidal Compounds)
 Section cross-reference(s): 73

IT 889869-73-2P 889869-74-3P

RL: DEV (Device component use); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)

(preparation of cyclopatinated fluorophenyl quinoxaline organometallic complex and their use as light-emitting element and $\,$

light-emitting device)

IT 148186-43-0P, 2,3-Bis(4-fluorophenyl)quinoxaline 223707-22-0P 870136-70-2P 889869-72-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of cyclopatinated fluorophenyl quinoxaline organometallic complex and their use as light-emitting element and light-emitting device)

REFERENCE COUNT:

THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 4 OF 14 HCAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 2006:564313 HCAPLUS Full-text

5

DOCUMENT NUMBER:

145:53427

TITLE:

Group 9 or 10 metal complexes,

electroluminescent devices having layer containing them, and use of the devices

INVENTOR(S): Inoue, Eiko; Seo, Satoshi; Shimogaki, Tomoko;

Abe, Hiroko

PATENT ASSIGNEE(S): Semiconductor Energy Laboratory Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 67 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
	JP 2006151887	A	20060615	JP 2004-346234	
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PRIOR	RITY APPLN. INFO.:			JP 2004-346234	
					200411
					30

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OTHER SOURCE(S): MARPAT 145:53427

GI

AB The complexes are represented by I (R1-R5 = H, halo, acyl, alkyl, alkoxy, aryl, cyano, heterocyclyl; Ar = aryl, heterocyclyl; M = group 9 or 10 element) or II (R21-R25 = any group given for R1-R5; Ar, M = same as above; n = 1 when M = group 10 element or 2 when M = group 9 element; L = monoanionic ligand having β -diketone structure, monoanionic bidentate ligand containing carboxy group or phenolic OH). Also claimed are electroluminescent apparatus having the electroluminescent devices and electronic instruments having the apparatus in the display. I or II emit phosphorescence and are also useful as sensitizers for fluorescent compds.

IT 848127-98-0P 853994-39-5P 870245-89-9P 870245-91-3P 870245-92-4P

RL: DEV (Device component use); MOA (Modifier or additive use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)

(preparation of group 9 or 10 metal arylquinoxaline complexes emitting phosphorescence and electroluminescent devices using them)

RN 848127-98-0 HCAPLUS

CN Iridium, $(2,4-pentanedionato-\kappa O,\kappa O')$ bis $[2-(3-phenyl-2-quinoxalinyl-\kappa N1)phenyl-\kappa C]-(9CI)$ (CA INDEX NAME)

PAGE 1-A

RN 853994-39-5 HCAPLUS

CN Iridium, bis[5-fluoro-2-[3-(4-fluorophenyl)-2-quinoxalinyl- κ N1]phenyl- κ C](2,4-pentanedionato- κ O2, κ O4)- (CA INDEX NAME)

PAGE 1-A

RN 870245-89-9 HCAPLUS

CN Iridium, bis[5-fluoro-2-[3-(4-fluorophenyl)-2-quinoxalinyl- κ N1]phenyl- κ C](2-pyridinecarboxylato- κ N1, κ O2)- (9CI) (CA INDEX NAME)

RN 870245-91-3 HCAPLUS

CN Iridium, bis[2-[3-(3,5-difluorophenyl)-2-quinoxalinyl- κ N1]-4,6-difluorophenyl- κ C](2,4-pentanedionato- κ O, κ O')-(9CI) (CA INDEX NAME)

PAGE 1-A

$$\begin{array}{c} F \\ \\ N \\ \\ \end{array}$$

RN 870245-92-4 HCAPLUS

CN Iridium, bis[2-[3-(3,5-difluorophenyl)-2-quinoxalinyl- κ N1]-4,6-difluorophenyl- κ C](2-pyridinecarboxylato- κ N1, κ O2)-(9CI) (CA INDEX NAME)

IT 848127-97-9P 848889-99-6P 870245-90-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of group 9 or 10 metal arylquinoxaline complexes emitting phosphorescence and electroluminescent devices using them)

RN 848127-97-9 HCAPLUS

CN Iridium, di- μ -chlorotetrakis[2-(3-phenyl-2-quinoxalinyl- κ N1)phenyl- κ C]di- (CA INDEX NAME)

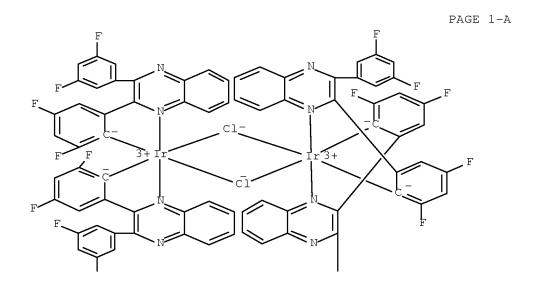
RN 848889-99-6 HCAPLUS

CN Iridium, di- μ -chlorotetrakis[5-fluoro-2-[3-(4-fluorophenyl)-2-quinoxalinyl- κ N1]phenyl- κ C]di- (CA INDEX NAME)

PAGE 1-A

RN 870245-90-2 HCAPLUS

CN Iridium, di- μ -chlorotetrakis[2-[3-(3,5-difluorophenyl)-2-quinoxalinyl- κ N1]-4,6-difluorophenyl- κ C]di- (9CI) (CA INDEX NAME)



CC 74-13 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)

Section cross-reference(s): 29

848127-98-0P 853994-39-5P 870245-89-9P

870245-91-3P 870245-92-4P

RL: DEV (Device component use); MOA (Modifier or additive use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)

(preparation of group 9 or 10 metal arylquinoxaline complexes emitting phosphorescence and electroluminescent devices using them)

ΙT 19802-70-1P 148186-43-0P, 2,3-Bis(4-fluorophenyl)quinoxaline 787640-67-9P 848127-97-9P 223707-22-0P

848889-99-6P 870136-70-2P 870245-90-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of group 9 or 10 metal arylquinoxaline complexes emitting phosphorescence and electroluminescent devices using them)

L12 ANSWER 5 OF 14 HCAPLUS COPYRIGHT 2008 ACS on STN

2005:1262621 HCAPLUS Full-text ACCESSION NUMBER:

DOCUMENT NUMBER: 144:29490

Light emitting element and light emitting device TITLE: INVENTOR(S): Ohsawa, Nobuharu; Abe, Hiroko; Inoue, Hideko;

Shitagaki, Satoko; Seo, Satoshi

PATENT ASSIGNEE(S): Semiconductor Energy Laboratory Co., Ltd., Japan

SOURCE: PCT Int. Appl., 196 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND DATE	APPLICATION NO.	DATE
WO 2005115061	A1 20051201	WO 2005-JP9310	200505 17
CH, CN, CO, GB, GD, GE, KP, KR, KZ, MW, MX, MZ, SC, SD, SE, UG, US, UZ, RW: BW, GH, GM, AM, AZ, BY, DE, DK, EE, NL, PL, PT,	CR, CU, CZ, DE, GH, GM, HR, HU, LC, LK, LR, LS, NA, NG, NI, NO, SG, SK, SL, SM, VC, VN, YU, ZA, KE, LS, MW, MZ, KG, KZ, MD, RU, ES, FI, FR, GB,	NA, SD, SL, SZ, TZ, UC TJ, TM, AT, BE, BG, CF GR, HU, IE, IS, IT, LT TR, BF, BJ, CF, CG, CT	G, ES, FI, E, KG, KM, G, MK, MN, I, RO, RU, I, TZ, UA, G, ZM, ZW, H, CY, CZ, I, LU, MC,
R: DE, FI, FR,	GB, NL	EP 2005-740951	200505 17
CN 1957645 JP 2006073992		CN 2005-80016049 < JP 2005-147413	200505 17 200505 19

August 4, 2006		10/390,703		
US 20070241667	A1	20071018	< US 2006-590703	
			<	200608 25
KR 2007015605	A	20070205	KR 2006-725371	200612
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JP 2007314541	A	20071206	JP 2007-146489	200706
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PRIORITY APPLN. INFO.:			JP 2004-151035 A	200405
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			JP 2004-226382 A	200408
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OTHER SOURCE(S):

MARPAT 144:29490

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 R^4

$$\begin{bmatrix} R^3 & R^4 \\ R^2 & & \\ & &$$

AB Light-emitting elements comprising a pair of electrodes (an anode and a cathode) wit a light-emitting layer between them are described in which the light-emitting layer includes an organometallic complex described by the general formulas I or II (R1-5 = H, halo, acyl, alkyl, alkoxyl, aryl, cyano, and/or heterocyclic groups; Ar = an aryl group having an electron-withdrawing group or a heterocyclic group having an electron-withdrawing group; M = a Group 9 or Group 10 element; n = 2 if M = Group 9 element; n = 1 if M = Group 10 element; and L = anionic ligand) and a compound that has a larger energy gap than the organometallic complex or a compound that has a larger ionization

ΙI

potential and a smaller electron affinity than the organometallic complex. Light-emitting devices using the light-emitting elements are also described.

IT 848127-98-0P 853994-39-5P 870245-89-9P

870245-91-3P 870245-92-4P

RL: DEV (Device component use); MOA (Modifier or additive use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)

(light-emitting elements employing organometallic compds.)

RN 848127-98-0 HCAPLUS

CN Iridium, $(2,4-pentanedionato-\kappa O,\kappa O')$ bis $[2-(3-phenyl-2-quinoxalinyl-\kappa N1)phenyl-\kappa C]-(9CI)$ (CA INDEX NAME)

PAGE 1-A

RN 853994-39-5 HCAPLUS

CN Iridium, bis[5-fluoro-2-[3-(4-fluorophenyl)-2-quinoxalinyl- κ N1]phenyl- κ C](2,4-pentanedionato- κ O2, κ O4)- (CA INDEX NAME)

PAGE 1-A

RN 870245-89-9 HCAPLUS

CN Iridium, bis[5-fluoro-2-[3-(4-fluorophenyl)-2-quinoxalinyl- κ N1]phenyl- κ C](2-pyridinecarboxylato- κ N1, κ O2)- (9CI) (CA INDEX NAME)

RN 870245-91-3 HCAPLUS

CN Iridium, bis[2-[3-(3,5-difluorophenyl)-2-quinoxalinyl- κ N1]-4,6-difluorophenyl- κ C](2,4-pentanedionato- κ O, κ O')- (9CI) (CA INDEX NAME)

PAGE 1-A

$$\begin{array}{c|c} F & F \\ \hline \\ N & \\ \hline \\ Ir3+ \\ \hline \end{array}$$

RN 870245-92-4 HCAPLUS

CN Iridium, bis $[2-[3-(3,5-difluoropheny1)-2-quinoxaliny1-\kappa N1]-4,6-difluoropheny1-\kappa C]$ (2-pyridinecarboxylato- κ N1, κ O2)- (9CI) (CA INDEX NAME)

RN 848889-99-6 HCAPLUS

CN Iridium, di- μ -chlorotetrakis[5-fluoro-2-[3-(4-fluorophenyl)-2-quinoxalinyl- κ N1]phenyl- κ C]di- (CA INDEX NAME)

PAGE 1-A

RN 870245-90-2 HCAPLUS

CN Iridium, di- μ -chlorotetrakis[2-[3-(3,5-difluorophenyl)-2-quinoxalinyl- κ N1]-4,6-difluorophenyl- κ C]di- (9CI) (CA INDEX NAME)

F F

IC ICM H05B033-14 ICS C09K011-06

CC 73-11 (Optical, Electron, and Mass Spectroscopy and Other Related Properties)

Section cross-reference(s): 29, 76

IT 848127-98-0P 853994-39-5P 870245-89-9P

870245-91-3P 870245-92-4P

RL: DEV (Device component use); MOA (Modifier or additive use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)

(light-emitting elements employing organometallic compds.)

IT 19802-70-1P 148186-43-0P, 2,3-Bis(4-fluorophenyl)quinoxaline 223707-22-0P 848127-97-9P 848889-99-6P

870136-70-2P 870245-90-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(light-emitting elements employing organometallic compds.)

REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR

THIS RECORD. ALL CITATIONS AVAILABLE IN

THE RE FORMAT

L12 ANSWER 6 OF 14 HCAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 2005:1149648 HCAPLUS <u>Full-text</u>

DOCUMENT NUMBER: 143:422468

TITLE: Preparation of N-containing heterocycle-di(2-

pyridyl)amine-iridium complexes and luminescent

materials using them

INVENTOR(S): Konno, Hideo

PATENT ASSIGNEE(S): National Institute of Advanced Industrial

Science & Technology, Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 30 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PAT	TENT NO.	KIND	DATE	APPLICATION NO.		DATE
					_	
JP	2005298483	А	20051027	JP 2005-61293		
						200503 04
				<		
PRIORITY	Y APPLN. INFO.:			JP 2004-76281	А	
						200403 17

<--

OTHER SOURCE(S): MARPAT 143:422468

GΙ

The title iridium complexes (I) [n = 0, 1; X1 = H, (un)substituted aryl, N-AΒ containing heterocyclyl; Z1, Z2, Y1, Q1 = a group of atoms necessary to form optionally substituted 5- or 6-membered ring optionally condensed to another ring; L1 = a single bond, a divalent group; Y1 = N or C atom; when Y1 is C atom, Q1 and Y1 are bonded to each other through a double bond; R1-R8 = H, substituent] are prepared by reaction of di(2-pyridyl)amine ligand (II) (R1-R8, n, X1 = same as above) with iridium chloride binuclear complexes (III) [Z3-Z6, Y2, Y3, Q2, Q3] = a group of atoms necessary to form optionallysubstituted 5- or 6-membered ring optionally condensed to another ring; L2, L3 = a single bond, a divalent group; when Y2 and Y3 are C atoms, the bond between C atom and Q3 and one between Q2 and Y2 are double bonds] under microwave irradiation These iridium complexes provide luminescent materials for luminescent devices with high brightness, high efficiency, and durability, materials for organic electroluminescent devices and electro-chemiluminescence (ECL) devices, luminescent sensors, photosensitizers, displays, fluorescent brighteners, photograph. materials, laser dyes, color filter dyes, optical communication, color conversion filter, back light, illumination, photosensitizing dyes, or various light sources. Thus, 200 mg bridged dimer (IV), 79 mg di(2-pyridyl)amine, and 25 mL 2-ethoxyethanol were added to a flask, irradiated in a microwave apparatus (Hitachi MR250) at 2,450 MHz for 15 min, cooled to room temperature, evaporated under reduced pressure to give a yellow solid which was dissolved in a mixture of ethanol and water, treated dropwise with a saturated aqueous solution of NH4PF6 to give, a yellow solid. The solid was recrystd. from CH2Cl2-hexane to give (2-phenylpyridine)[di(2pyridyl)amine]iridium complex (V). A solution of V in THF showed strong green luminescence at λ max of 482 and 512 nm.

IT 868131-65-1P

RL: DEV (Device component use); PRP (Properties); SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)

(preparation of N-containing heterocycle-di(2-pyridyl)amine-iridium complexes as luminescent materials)

^{*} STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

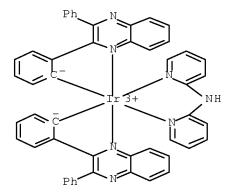
RN 868131-65-1 HCAPLUS CN

Iridium(1+), bis[2-(3-phenyl-2-quinoxalinyl- κ N1)phenyl- κ C][N-2-pyridinyl-2-pyridinamine- κ N]-, hexafluorophosphate(1-) (9CI) (CA INDEX NAME)

CM1

CRN 868131-64-0 CMF C50 H35 Ir N7

CCI CCS



CM 2

CRN 16919-18-9

CMF F6 P CCI CCS

ΙT 848127-97-9

RL: RCT (Reactant); RACT (Reactant or reagent) (preparation of N-containing heterocycle-di(2-pyridyl)amine-iridium complexes as luminescent materials)

848127-97-9 HCAPLUS RN

CN Iridium, $di-\mu$ -chlorotetrakis[2-(3-phenyl-2-quinoxalinyl- κ N1)phenyl- κ C]di- (CA INDEX NAME)

```
ICM C07F015-00
IC
    ICS C09K011-06; H05B033-14
    29-13 (Organometallic and Organometalloidal Compounds)
CC
    Section cross-reference(s): 76
    868131-25-3P
                  868131-27-5P
ΤT
                                  868131-29-7P
                                                 868131-31-1P
                  868131-35-5P
    868131-33-3P
                                  868131-37-7P
                                                 868131-39-9P
    868131-41-3P
                                  868131-45-7P
                   868131-43-5P
                                                 868131-47-9P
    868131-49-1P
                   868131-51-5P
                                  868131-53-7P
                                                 868131-54-8P
    868131-56-0P
                   868131-58-2P
                                  868131-59-3P
                                                 868131-61-7P
    868131-63-9P 868131-65-1P 868131-67-3P
                                               868131-69-5P
    868131-71-9P
                   868131-73-1P
                                  868131-75-3P
    RL: DEV (Device component use); PRP (Properties); SPN (Synthetic
    preparation); TEM (Technical or engineered material use); PREP
     (Preparation); USES (Uses)
        (preparation of N-containing heterocycle-di(2-pyridyl)amine-iridium
        complexes as luminescent materials)
ΙT
    1202-34-2, Di(2-pyridyl)amine 6654-69-9, Bis(3-methyl-2-
    pyridyl)amine 10428-50-9, Tri(2-pyridyl)amine 14192-97-3,
    N, N-Di(2-pyridyl) phenylamine 57175-14-1 343978-72-3
    391611-77-1 417705-49-8
                              435294-69-2
                                            603109-48-4
                                                          632326-35-3
    632327-35-6 632327-36-7
                                632327-37-8
                                              760997-15-7 760997-17-9
    848127-97-9
                  852609-81-5
                                861348-71-2,
    N, N-Di(2-pyridyl)(2-hydroxyphenyl)amine
                                              868131-76-4
                                                            868131-77-5
    868131-78-6
                 868131-79-7
                               868131-80-0
                                              868131-81-1
                                                            868131-82-2
    RL: RCT (Reactant); RACT (Reactant or reagent)
        (preparation of N-containing heterocycle-di(2-pyridyl)amine-iridium
        complexes as luminescent materials)
```

L12 ANSWER 7 OF 14 HCAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 2005:963628 HCAPLUS <u>Full-text</u>

DOCUMENT NUMBER: 143:275296

TITLE: Organometallic compound containing quinoxaline

structure and light emitting element

INVENTOR(S): Fujii, Hiroyuki; Hirao, Toshikazu; Sakurai,

Hidehiro; Mao, Lisheng; Tani, Kazuyasu

PATENT ASSIGNEE(S): Japan

SOURCE: U.S. Pat. Appl. Publ., 19 pp.

CODEN: USXXCO

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE

				-
US 20050191527	A1	20050901	US 2005-64123	200502 23
JP 2005239648	A	20050908	< JP 2004-52742	200402 27
PRIORITY APPLN. INFO.:			< JP 2004-52742	A 200402 27
			<	

OTHER SOURCE(S): MARPAT 143:275296

$$\begin{bmatrix} R1 & & & & & \\ R1 & & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ & & & & \\ &$$

- Organometallic compds. comprising a quinoxaline structure are described by the general formula I and II (M = a monovalent to trivalent metal; L and K = ligands; E = a cyclic structure, R1-5 = independently selected H or arbitrary substituents; Ar1-2 = independently selected (un)substituted aryl groups; m = 1-3; n = 0-3; n' = 0-2; p = 0-2; m + n + p = 2-5; and m n' = 1-3). Lightemitting devices are also described which employ the compds.

 II 848127-98-0P 853994-39-5P
 - RL: DEV (Device component use); MOA (Modifier or additive use); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(organometallic compds. containing quinoxaline structures and light-emitting elements using them)

- RN 848127-98-0 HCAPLUS
- CN Iridium, $(2,4-pentanedionato-\kappa O,\kappa O')$ bis $[2-(3-phenyl-2-quinoxalinyl-\kappa N1)phenyl-\kappa C]-(9CI)$ (CA INDEX NAME)

PAGE 1-A

RN 853994-39-5 HCAPLUS

CN Iridium, bis[5-fluoro-2-[3-(4-fluorophenyl)-2-quinoxalinyl- κ N1]phenyl- κ C](2,4-pentanedionato- κ O2, κ O4)- (CA INDEX NAME)

PAGE 1-A

IT 863714-58-3P 863714-60-7P 863714-61-8P 863714-62-9P

RL: DEV (Device component use); MOA (Modifier or additive use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)

(organometallic compds. containing quinoxaline structures and light-emitting elements using them)

RN 863714-58-3 HCAPLUS

CN Iridium, bis[5-methyl-2-[3-(4-methylphenyl)-2-quinoxalinyl- κ N1]phenyl- κ C](2,4-pentanedionato- κ O, κ O')-(9CI) (CA INDEX NAME)

PAGE 1-A

RN 863714-60-7 HCAPLUS

CN Iridium, bis[5-methoxy-2-[3-(4-methoxyphenyl)-2-quinoxalinyl- κ N1]phenyl- κ C](2,4-pentanedionato- κ O, κ O')- (9CI) (CA INDEX NAME)

PAGE 1-A

RN 863714-61-8 HCAPLUS

CN Iridium, tris[2-(3-phenyl-2-quinoxalinyl- κ N1)phenyl- κ C]- (9CI) (CA INDEX NAME)

RN 863714-62-9 HCAPLUS

CN Iridium, tris[5-fluoro-2-[3-(4-fluorophenyl)-2-quinoxalinyl- κ N1]phenyl- κ C]- (9CI) (CA INDEX NAME)

IT 848127-97-9P 848889-99-6P 863714-57-2P 863714-59-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

RN 848127-97-9 HCAPLUS

CN Iridium, di- μ -chlorotetrakis[2-(3-phenyl-2-quinoxalinyl- κ N1)phenyl- κ C]di- (CA INDEX NAME)

RN 848889-99-6 HCAPLUS

CN Iridium, di- μ -chlorotetrakis[5-fluoro-2-[3-(4-fluorophenyl)-2-quinoxalinyl- κ N1]phenyl- κ C]di- (CA INDEX NAME)

PAGE 1-A

RN 863714-57-2 HCAPLUS

CN Iridium, di- μ -chlorotetrakis[5-methyl-2-[3-(4-methylphenyl)-2-quinoxalinyl- κ N1]phenyl- κ C]di- (9CI) (CA INDEX NAME)

PAGE 1-A

RN 863714-59-4 HCAPLUS

CN Iridium, di- μ -chlorotetrakis[5-methoxy-2-[3-(4-methoxyphenyl)-2-quinoxalinyl- κ N1]phenyl- κ C]di- (9CI) (CA INDEX NAME)

PAGE 1-A

IC ICM B32B009-00

INCL 428917000; 428690000

CC 73-11 (Optical, Electron, and Mass Spectroscopy and Other Related Properties)

Section cross-reference(s): 29, 76

IT 848127-98-0P 853994-39-5P

RL: DEV (Device component use); MOA (Modifier or additive use); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(organometallic compds. containing quinoxaline structures and light-emitting elements using them)

IT 863714-58-3P 863714-60-7P 863714-61-8P 863714-62-9P

RL: DEV (Device component use); MOA (Modifier or additive use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)

August 4, 2008 10/590,703 449-46-7P, 2-(4-Fluorophenyl)quinoxaline 1684-14-6P, 2,3-Diphenylquinoxaline 3719-84-4P 5021-43-2P, 2-Phenylquinoxaline 7248-16-0P, 2,3-Bis(4methoxyphenyl)quinoxaline 36305-53-0P 148186-43-0P 810681-91-5P 810681-92-6P 810681-93-7P 810681-94-8P 810681-95-9P 810681-96-0P 810681-97-1P 810681-98-2P 810681-99-3P 810682-00-9P 848127-97-9P 848889-99-6P 863659-74-9P 863714-57-2P 863714-59-4P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (organometallic compds. containing quinoxaline structures and light-emitting elements using them) L12 ANSWER 8 OF 14 HCAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 2005:523471 HCAPLUS Full-text DOCUMENT NUMBER: 143:68073 Organic metal complex and light-emitting device TITLE: employing it INVENTOR(S): Inoue, Hideko; Seo, Satoshi; Shitagaki, Satoko; Abe, Hiroko

Semiconductor Energy Laboratory Co., Ltd., Japan PATENT ASSIGNEE(S):

SOURCE: PCT Int. Appl., 77 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.				KIND		DATE		APPLICATION NO.					DATE			
WO	 2005054261				A1		20050616							200411 29		
	W: RW:	CH, GB, KR, MX, SE, VC, BW, AM, DE,	CN, GD, KZ, MZ, SG, VN, GH, AZ, DK, PT,	CO, GE, LC, NA, SK, YU, GM, BY, EE,	CR, GH, LK, NI, SL, ZA, KE, KG, ES,	CU, GM, LR, NO, SY, ZM, LS, KZ, FI,	MW, MD, FR, SK,	DE, HU, LT, OM, TM, MZ, RU, GB, TR,	DK, ID, LU, PG, TN, NA, TJ, GR, BF,	DM, IL, LV, PH, TR, SD, TM, HU,	DZ, IN, MA, PL, TT, SL, AT, IE,	EC, IS, MD, PT, TZ, SZ, BE, IS,	EE, JP, MG, RO, UA, TZ, BG, IT,	EG, KE, MK, RU, UG, CH, LU,	ES, KG, MN, SC, US, ZM, CY, MC,	FI, KP, MW, SD, UZ, ZW, CZ, NL,
EP	1690	GQ, GW, ML, MR, NE, SN, TD, TG 1690866 A1 20060816 EP 2004-799935							200411 29							
JP	R: 3810				NL, B2		20060816		JP 2005-516006				2	00411		
CN	1890255		A	A 20070		0103	CN 2		2004-80035633				2	00411 9		

	00054400	<		
A1	20051103	US 2004-23043		200412
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		<		20
В2	20070703			
A1	20070913	US 2007-797532		
				200705
				0 4
		·	-	
		JP 2003-403822	А	200312
				02
		<		02
		WO 2004-JP18079	W	
				200411
				29
		<		
		US 2004-23043	A3	000410
				200412 28
		<		20
		в2 20070703	A1 20051103 US 2004-23043 B2 20070703 A1 20070913 US 2007-797532 JP 2003-403822 WO 2004-JP18079	A1 20051103 US 2004-23043 < B2 20070703 A1 20070913 US 2007-797532 < JP 2003-403822 A < WO 2004-JP18079 W < US 2004-23043 A3

MARPAT 143:68073

OTHER SOURCE(S):

GI

$$R^3$$
 R^4
 R^5
 R^5
 R^4
 R^5
 R^4

AB An organic metal complex is characterized by having a structure represented by the general formula (I) below. In the formula, R1-R5 resp. represent a hydrogen atom, a halogen element, an acyl group, an alkyl group, an alkoxyl group, an aryl group, a cyano group or a heterocyclic residue; Ar represents an aryl group having an electron-withdrawing substituent or a heterocyclic residue having an electron-withdrawing substituent; and M represents a group IX element or a group X element.

IT 848127-98-0P 853994-39-5P

RL: DEV (Device component use); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)

(organic metal complex and light-emitting device employing it)

RN 848127-98-0 HCAPLUS

CN Iridium, $(2,4-pentanedionato-\kappa O,\kappa O')$ bis $[2-(3-phenyl-2-quinoxalinyl-\kappa N1)phenyl-\kappa C]-(9CI)$ (CA INDEX NAME)

PAGE 1-A

RN 853994-39-5 HCAPLUS

CN Iridium, bis[5-fluoro-2-[3-(4-fluorophenyl)-2-quinoxalinyl- κ N1]phenyl- κ C](2,4-pentanedionato- κ O2, κ O4)- (CA INDEX NAME)

PAGE 1-A

ICM C07F015-00 IC ICS C09K011-06; H05B033-14

CC 73-11 (Optical, Electron, and Mass Spectroscopy and Other Related Properties)

Section cross-reference(s): 29

848127-98-0P 853994-39-5P ΙT

> RL: DEV (Device component use); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)

(organic metal complex and light-emitting device employing it) REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 9 OF 14 HCAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 2004:1044364 HCAPLUS Full-text

DOCUMENT NUMBER: 142:316925

TITLE: Synthesis and photoluminescence of a new red phosphorescent iridium(III) quinoxaline complex

AUTHOR(S): Zhang, Guo Lin; Liu, Ze Hua; Guo, Hai Qing

State Key Laboratory of Rare Earth Materials CORPORATE SOURCE: Chemistry and Applications, College of Chemistry and Molecular Engineering, Peking University,

Beijing, 100871, Peop. Rep. China

SOURCE: Chinese Chemical Letters (2004),

15(11), 1349-1352

CODEN: CCLEE7; ISSN: 1001-8417

PUBLISHER: Chinese Chemical Society

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 142:316925

AB A new cyclometalated iridium(III) complex with the formula [Ir(DPQ)2(acac)] (DPQ = 2,3-diphenylquinoxaline; acac = acetylacetone) was prepared The structure of the complex was confirmed by elemental anal. (EA), 1H NMR, and mass spectroscopy (MS). The UV-vis absorption and photoluminescent properties of the complex were investigated.

IT 848127-98-0P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)

(synthesis and photoluminescence of cyclometalated diphenylquinoxaline iridium acetylacetone complex)

RN 848127-98-0 HCAPLUS

CN Iridium, $(2,4-pentanedionato-\kappa O,\kappa O')$ bis $[2-(3-phenyl-2-quinoxalinyl-\kappa N1)phenyl-\kappa C]-(9CI)$ (CA INDEX NAME)

PAGE 1-A

IT 848127-97-9P

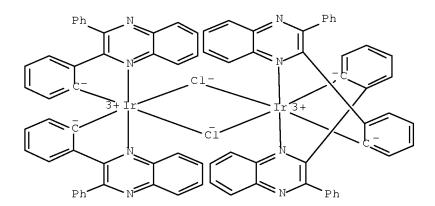
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);

RACT (Reactant or reagent)

(synthesis and photoluminescence of cyclometalated diphenylquinoxaline iridium acetylacetone complex)

RN 848127-97-9 HCAPLUS

CN Iridium, di- μ -chlorotetrakis[2-(3-phenyl-2-quinoxalinyl- κ N1)phenyl- κ C]di- (CA INDEX NAME)



CC 29-13 (Organometallic and Organometalloidal Compounds)

Section cross-reference(s): 73

IT 848127-98-0P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)

(synthesis and photoluminescence of cyclometalated diphenylquinoxaline iridium acetylacetone complex)

IT 1684-14-6P, 2,3-Diphenylquinoxaline 848127-97-9P

9

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(synthesis and photoluminescence of cyclometalated diphenylquinoxaline iridium acetylacetone complex)

REFERENCE COUNT:

THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 10 OF 14 HCAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 2000:614376 HCAPLUS <u>Full-text</u>

DOCUMENT NUMBER: 133:321984

TITLE: Effects of the nature of the ligand environment

and metal center on the optical and

electrochemical properties of platinum(II) and
palladium(II) ethylenediamine complexes with

heterocyclic cyclometalated ligands

AUTHOR(S): Kulikova, M. V.; Balashev, K. P.; Kvam, P.-I.;

Songstad, J.

CORPORATE SOURCE: Gertzen Russian State Pedagogical University,

St. Petersburg, Russia

SOURCE: Russian Journal of General Chemistry

(Translation of Zhurnal Obshchei Khimii) (

2000), 70(2), 163-170

CODEN: RJGCEK; ISSN: 1070-3632

PUBLISHER: MAIK Nauka/Interperiodica Publishing

DOCUMENT TYPE: Journal LANGUAGE: English

AB Mixed-ligand cyclometalated complexes [M(C.cxa.N)en]+ (M = Pt(II), Pd(II); C.cxa.N is a cyclometalating ligand on the basis of 2-(2'-thienyl)pyridine, 2-phenylpyridine, 2,6-diphenylpyridine, 2,3-diphenylpyrazine, 2,3-diphenylquinoxaline, and benzo(h)quinoline; en = ethylenediamine) were synthesized and characterized by 1H and 13C NMR, electron absorption and emission spectroscopy, and cyclic voltammetry. It was found that the LUMO is predominantly localized in the "N-imine" part of the (C.cxa.N) ligand and that the optical and electrochem. properties of the complexes are very sensitive to changes in this part of the ligand. "Mild" structural changes in the (C.cxa.N) ligands (introduction of various substituents) produce no such effect. The increase in the energy of the lowest excited state and the anodic shifts of the oxidation potentials of the complexes in going from palladium to platinum are explained in terms of enhanced stabilization of palladium 4d orbitals as compared to platinum 5d orbitals.

IT 303045-45-6P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)

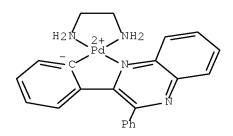
(crystal structure; effects of nature of ligand environment and metal center on optical and electrochem. properties of platinum and palladium ethylenediamine complexes with heterocyclic cyclometalated ligands)

RN 303045-45-6 HCAPLUS

CN Palladium(1+), (1,2-ethanediamine- κ N, κ N')[2-(3-phenyl-2-quinoxalinyl- κ N1)phenyl- κ C]-, (SP-4-2)-, chloride, compd. with methanol (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 266352-74-3 CMF C22 H21 N4 Pd . C1 CCI CCS



● C1-

CM 2

CRN 67-56-1 CMF C H4 O

Н3С—ОН

47

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)

(effects of nature of ligand environment and metal center on optical and electrochem. properties of platinum and palladium ethylenediamine complexes with heterocyclic cyclometalated ligands)

RN 266352-76-5 HCAPLUS

CN Platinum(1+), (1,2-ethanediamine- κ N, κ N')[2-(3-phenyl-2-quinoxalinyl- κ N1)phenyl- κ C]-, (SP-4-2)-, perchlorate (9CI) (CA INDEX NAME)

CM 1

CRN 266352-75-4 CMF C22 H21 N4 Pt CCI CCS

CM 2

CRN 14797-73-0 CMF Cl O4

RN 303045-40-1 HCAPLUS

CN Palladium(1+), (1,2-ethanediamine- κ N, κ N')[2-(3-phenyl-2-quinoxalinyl- κ N1)phenyl- κ C]-, (SP-4-2)-, perchlorate (9CI) (CA INDEX NAME)

CM 1

CRN 303045-39-8 CMF C22 H21 N4 Pd CCI CCS

CM 2

CRN 14797-73-0 CMF Cl O4

CC 29-13 (Organometallic and Organometalloidal Compounds)

Section cross-reference(s): 72

IT 303045-45-6P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)

(crystal structure; effects of nature of ligand environment and metal center on optical and electrochem. properties of platinum and palladium ethylenediamine complexes with heterocyclic cyclometalated ligands)

IT 164533-54-4P 167647-75-8P 223732-46-5P 223732-48-7P 255837-37-7P 266352-76-5P 303045-26-3P 303045-34-3P 303045-36-5P 303045-40-1P 303045-42-3P 303045-44-5P RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)

(effects of nature of ligand environment and metal center on optical and electrochem. properties of platinum and palladium ethylenediamine complexes with heterocyclic cyclometalated ligands)

REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 11 OF 14 HCAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 2000:211471 HCAPLUS Full-text

DOCUMENT NUMBER: 132:321975

TITLE: Synthesis and properties of palladium(II) and

platinum(II) (2,3-diphenylquinoxalinato-

C, N) ethylenediamine complexes

AUTHOR(S): Balashev, K. P.; Kulikova, M. V.; Kvam, P.-I.;

Songstad, J.

CORPORATE SOURCE: Gertzen Russian State Pedagogical University,

St. Petersburg, Russia

SOURCE: Russian Journal of General Chemistry

(Translation of Zhurnal Obshchei Khimii) (

1999), 69(8), 1348-1349

CODEN: RJGCEK; ISSN: 1070-3632

PUBLISHER: MAIK Nauka/Interperiodica Publishing

DOCUMENT TYPE: Journal LANGUAGE: English

Palladium(II) and platinum(II) diphenylquinoxalinato complexes, [M(C-N)Cl]2 (I; M = Pt, Pd, C-N = deprotonated form of 2,3-diphenylquinoxaline) underwent ligand substitution reaction with ethylenediamine (en) to give [M(C-N)(en)]X (M = Pd, X = Cl; M = Pt, X = ClO4, resp.). I (M = Pt) was prepared from [PtCl4][NBu4] and HC-N in CH2Cl2 at 50°.

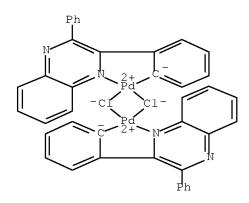
IT 266352-77-6

RL: RCT (Reactant); RACT (Reactant or reagent)

(ligand substitution reaction with ethylenediamine)

RN 266352-77-6 HCAPLUS

CN Palladium, di- μ -chlorobis[2-(3-phenyl-2-quinoxalinyl- κ N1)phenyl- κ C]di- (9CI) (CA INDEX NAME)



IT 266352-78-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and ligand substitution reaction with ethylenediamine)

RN 266352-78-7 HCAPLUS

CN Platinum, $di-\mu$ -chlorobis[2-(3-phenyl-2-quinoxalinyl- κ N1)phenyl- κ C]di- (9CI) (CA INDEX NAME)

ΙT

RN 266352-74-3 HCAPLUS

CN Palladium(1+), (1,2-ethanediamine- κ N, κ N')[2-(3-phenyl-2-quinoxalinyl- κ N1)phenyl- κ C]-, chloride, (SP-4-2)- (9CI) (CA INDEX NAME)

● c1-

RN 266352-76-5 HCAPLUS

CN Platinum(1+), (1,2-ethanediamine- κ N, κ N')[2-(3-phenyl-2-quinoxalinyl- κ N1)phenyl- κ C]-, (SP-4-2)-, perchlorate (9CI) (CA INDEX NAME)

CM 1

CRN 266352-75-4 CMF C22 H21 N4 Pt CCI CCS

CM 2

CRN 14797-73-0 CMF C1 O4

```
CC
     29-13 (Organometallic and Organometalloidal Compounds)
IT
     266352-77-6
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (ligand substitution reaction with ethylenediamine)
     266352-78-7P
ΤТ
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);
     RACT (Reactant or reagent)
        (preparation and ligand substitution reaction with ethylenediamine)
     266352-74-3P 266352-76-5P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (preparation of)
REFERENCE COUNT:
                               THERE ARE 6 CITED REFERENCES AVAILABLE FOR
                               THIS RECORD. ALL CITATIONS AVAILABLE IN
                               THE RE FORMAT
L12 ANSWER 12 OF 14 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER:
                         2000:200721 HCAPLUS Full-text
DOCUMENT NUMBER:
                         133:4789
                         Bromination and nitration reactions of
TITLE:
                         metallated (Ru and Os) multiaromatic ligands and
                         crystal structures of selected products
AUTHOR(S):
                         Clark, Alex M.; Rickard, Clifton E. F.; Roper,
                         Warren R.; Wright, L. James
                         Department of Chemistry, The University of
CORPORATE SOURCE:
                         Auckland, Auckland, 92019, N. Z.
                         Journal of Organometallic Chemistry (
SOURCE:
                         2000), 598(2), j262-275
                         CODEN: JORCAI; ISSN: 0022-328X
PUBLISHER:
                         Elsevier Science S.A.
                         Journal
DOCUMENT TYPE:
LANGUAGE:
                         English
OTHER SOURCE(S):
                         CASREACT 133:4789
     Three N-containing aromatic heterocycles, 2-(1'-naphthyl)pyridine, 2-
     phenylquinoline, and 2,3-diphenylquinoxaline, were mercurated in the naphthyl
     or Ph ring 2-position and then symmetrized to form the Hg compds. Ar2Hg (Ar =
     Nppy (3), Phqn (1) or Dpqx (5), resp.). These reagents are suitable for trans-
     metalation and reaction with MHCl(CO)(PPh3)3 affords the complexes M(n2-C,N-C)
     Ar)C1(CO)(PPh3)2, (6, M = Ru, Ar = Nppy; 7, M = Os, Ar = Nppy; 8, M = Ru, Ar =
     Phqn; 9, M = Os, Ar = Phqn; 10, M = Ru, Ar = Dpqx; 11, M = Os, Ar = Dpqx) in
     which each product features an aryl ligand that forms a strongly chelated
     five-membered ring through coordination of the heterocyclic N atom.
     chloride ligand in each of the complexes 6-11 can be replaced by di-Me
     dithiocarbamate to give ultimately the mono-PPh3 complexes, M(\eta 2-Ar)(\eta 2-Ar)
     S2CNMe2)(CO)(PPh3) (12, M = Ru, Ar = Nppy; 13, M = Os, Ar = Nppy; 14, M = Ru,
     Ar = Phqn; 15, M = Os, Ar = Phqn; 16, M = Ru, Ar = Dpqx; 17, M = Os, Ar =
     Dpgx). Similarly, compound 10 when treated with Na(acac) gives Ru(\eta 2-
     Dpqx)(\eta2- acac)(CO)(PPh3) (18), while treatment with HO2CCF3 gives Ru(\eta2-
     Dpqx)(O2CCF3)(CO)(PPh3)2 (19). Many of these complexes are very robust,
     making them suitable for electrophilic aromatic substitution reactions under
     harsh conditions. In each case, the presence of the metal had both an
     activating and a directing effect on the aryl ring to which it was bonded.
     Bromination or nitration reactions, both of which are not normally possible
     with organometallic substrates, were carried out successfully, giving rise to
     monobrominated or dinitrated products, resp. The following compds. were
     characterized, M(\eta 2-Ar-4-Br)Cl(CO)(PPh3)2(20, M = Ru, Ar = Phqn; 21, M = Os,
     Ar = Phqn; 22, M = Ru, Ar = Dpqx; 24, M = Os, Ar = Dpqx), M(\eta 2-Dpqx-4-Br)(\eta 2-Dpqx-4-Br)
     S2CNMe2) (CO) (PPh3) (23, M = Ru; 25, M = Os), Os(\eta2-Ar)Cl(CO) (PPh3)2 (26, Ar =
```

Nppy-6,8-(NO2)2; 27, Ar = Phqn-4,6-(NO2)2). Crystal structures of compds. 7, 12, 15, 18, 19, 21, 23 and 25 were determined

IT 270252-38-5P 270252-39-6P 270252-44-3P

270252-46-5P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)

(preparation and crystal structure of)

RN 270252-38-5 HCAPLUS

CN Osmium, carbonyl(2,4-pentanedionato- κ O, κ O')[2-(3-phenyl-2-quinoxalinyl- κ N1)phenyl- κ C](triphenylphosphine)-, (OC-6-25)- (9CI) (CA INDEX NAME)

R---- C=== 0

RN 270252-39-6 HCAPLUS

CN Ruthenium, carbonyl[2-(3-phenyl-2-quinoxalinyl- κ N1)phenyl- κ C](trifluoroacetato- κ O)bis(triphenylphosphine)-, (OC-6-15)- (9CI) (CA INDEX NAME)

RN 270252-44-3 HCAPLUS

CN Ruthenium, [4-bromo-2-(3-phenyl-2-quinoxalinyl- κ N1)phenyl- κ C]carbonyl(dimethylcarbamodithioato- κ S, κ S')(triphenylphosphine)-, (OC-6-52)-, compd. with dichloromethane (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 270252-43-2

CMF C42 H33 Br N3 O P Ru S2

CCI CCS

CM 2

CRN 75-09-2 CMF C H2 C12

C1-CH2-C1

RN 270252-46-5 HCAPLUS

CN Osmium, [4-bromo-2-(3-phenyl-2-quinoxalinyl- κ N1)phenyl- κ C]carbonyl(dimethylcarbamodithioato- κ S, κ S')(triphenylphosphine)-, (OC-6-52)- (9CI) (CA INDEX NAME)

(preparation and symmetrization of)

RN 270252-21-6 HCAPLUS

CN Mercury, chloro[2-(3-phenyl-2-quinoxalinyl- κ N1)phenyl- κ C]- (9CI) (CA INDEX NAME)

RN 270252-37-4 HCAPLUS

CN Osmium, carbonyl(dimethylcarbamodithioato- κ S, κ S')[2-(3-phenyl-2-quinoxalinyl- κ N1)phenyl- κ C](triphenylphosphine)-, (OC-6-52)- (9CI) (CA INDEX NAME)

RN 270252-42-1 HCAPLUS

CN Ruthenium, [4-bromo-2-(3-phenyl-2-quinoxalinyl- κ N1)phenyl- κ C]carbonylchlorobis(triphenylphosphine)-, (OC-6-52)- (9CI) (CA INDEX NAME)

RN 270252-45-4 HCAPLUS

CN Osmium, [4-bromo-2-(3-phenyl-2-quinoxalinyl- κ N1)phenyl- κ C]carbonylchlorobis(triphenylphosphine)-, (OC-6-52)- (9CI) (CA INDEX NAME)

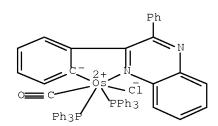
IT 270252-28-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation, coordinative metathesis with dithiocarbamate and ligand bromination)

RN 270252-28-3 HCAPLUS

CN Osmium, carbonylchloro[2-(3-phenyl-2-quinoxalinyl- κ N1)phenyl- κ C]bis(triphenylphosphine)-, (OC-6-52)- (9CI) (CA INDEX NAME)



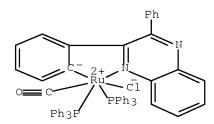
IT 270252-27-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation, coordinative metathesis with dithiocarbamate, coordinative condensation reactions with acetylacetone and trifluoroacetic acid and ligand bromination)

RN 270252-27-2 HCAPLUS

CN Ruthenium, carbonylchloro[2-(3-phenyl-2-quinoxalinyl- κ N1)phenyl- κ C]bis(triphenylphosphine)-, (OC-6-52)- (9CI) (CA INDEX NAME)



AUTHOR(S):

```
29-13 (Organometallic and Organometalloidal Compounds)
     Section cross-reference(s): 75
     270252-29-4P 270252-34-1P 270252-38-5P
ΙT
     270252-39-6P 270252-44-3P 270252-46-5P
     270252-49-8P
     RL: PRP (Properties); SPN (Synthetic preparation); PREP
     (Preparation)
        (preparation and crystal structure of)
ΙT
     119399-90-5P, 2-(2-Quinolinyl)phenylmercury chloride 270252-19-2P,
     1-(2-Pyridinyl)-2-naphthylmercury chloride 270252-21-6P,
     (2-(3-Phenyl-2-quinoxalinyl)phenyl)mercury chloride
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);
     RACT (Reactant or reagent)
        (preparation and symmetrization of)
     270252-18-1P, Bis(2-(2-quinolinyl)phenyl)mercury 270252-20-5P,
ΙT
     Bis(1-(2-pyridinyl)-2-naphthyl)mercury 270252-22-7P,
     Bis(2-(3-phenyl-2-quinoxalinyl)phenyl)mercury
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);
     RACT (Reactant or reagent)
        (preparation and transmetalation with osmium and ruthenium complexes)
ΙT
     270252-30-7P
                    270252-31-8P 270252-36-3P
     270252-37-4P
                    270252-40-9P 270252-42-1P
     270252-45-4P
                    270252-47-6P
                                   270252-48-7P
     RL: SPN (Synthetic preparation); PREP (Preparation)
        (preparation of)
ΙT
     270252-25-0P 270252-28-3P
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);
     RACT (Reactant or reagent)
        (preparation, coordinative metathesis with dithiocarbamate and ligand
        bromination)
     270252-27-2P
ΙT
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);
     RACT (Reactant or reagent)
        (preparation, coordinative metathesis with dithiocarbamate,
        coordinative condensation reactions with acetylacetone and
        trifluoroacetic acid and ligand bromination)
REFERENCE COUNT:
                         30
                               THERE ARE 30 CITED REFERENCES AVAILABLE
                               FOR THIS RECORD. ALL CITATIONS AVAILABLE
                               IN THE RE FORMAT
L12 ANSWER 13 OF 14 HCAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER:
                         1991:62321 HCAPLUS Full-text
DOCUMENT NUMBER:
                         114:62321
ORIGINAL REFERENCE NO.: 114:10698h, 10699a
TITLE:
                        Cyclometalated compounds. V. Double
                         cyclopalladation of diphenylpyrazines and
                        related ligands
```

Steel, Peter J.; Caygill, Graham B.

CORPORATE SOURCE: Chem. Dep., Univ. Canterbury, Christchurch, N.

Ζ.

SOURCE: Journal of Organometallic Chemistry (

1990), 395(3), 359-73

CODEN: JORCAI; ISSN: 0022-328X

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 114:62321

GΙ

AB 2,3-Diphenylpyrazine and 4 structurally related ligands have each been singly and doubly cyclopalladated and the products characterized by 1H and 13C NMR studies of their acetylacetonate complexes. The structure of a doubly cyclometalated Pd(acac) complex (I) of 2,3-diphenylpyrazine has been determined by an x-ray diffraction study. A strong steric interaction between the 2 cyclopalladated Ph rings is relieved by twisting; the 2 chelate ring mean-planes are mutually inclined at an angle of 19.6(5)°.

IT 131259-91-1P

RN 131259-91-1 HCAPLUS

CN Palladium, (2,4-pentanedionato-0,0')[2-(3-phenyl-2-quinoxalinyl)phenyl]-, (SP-4-3)- (9CI) (CA INDEX NAME)

CC 29-13 (Organometallic and Organometalloidal Compounds)

Section cross-reference(s): 75

IT 131259-88-6P 131259-90-0P 131259-91-1P 131259-92-2P 131259-93-3P 131259-94-4P 131259-95-5P 131259-96-6P

131259-97-7P 131612-44-7P

L12 ANSWER 14 OF 14 HCAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 1975:579265 HCAPLUS Full-text DOCUMENT NUMBER: 83:179265

ORIGINAL REFERENCE NO.: 83:28161a,28164a

TITLE: Cyclometallation reactions. XIII. Reactions of

phenyl-substituted heterocyclic nitrogen-donor

ligands

AUTHOR(S): Bruce, Michael I.; Goodall, Brian L.; Matsuda,

Isamu

CORPORATE SOURCE: Dep. Inorg. Chem., Univ. Bristol, Bristol, UK

SOURCE: Australian Journal of Chemistry (1975

), 28(6), 1259-64

CODEN: AJCHAS; ISSN: 0004-9425

DOCUMENT TYPE: Journal LANGUAGE: English

GI For diagram(s), see printed CA Issue.

AB The preparation of metalated complexes of Mn or Re derived from 2-phenylpyridine, 1,4-diphenylquinoxaline, 1-phenylpyrazole, 4-phenylpyrimidine, 1,4-diphenylphthalazine and 2,5-diphenyloxazole is described. Thus, heating 2-phenylpyridine with MnMe(CO)5 gave I.

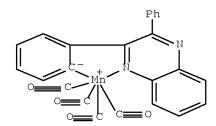
IT 57522-13-1P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

RN 57522-13-1 HCAPLUS

CN Manganese, tetracarbonyl[2-(3-phenyl-2-quinoxalinyl)phenyl]-, (OC-6-23)- (9CI) (CA INDEX NAME)



CC 29-11 (Organometallic and Organometalloidal Compounds)

IT 39046-05-4P 57522-10-8P 57522-11-9P 57522-12-0P 57522-13-1P 57522-14-2P 57522-15-3P 57522-16-4P

57522-13-1P 57522-14-2P 57522-15-3P 57522-16-4P 57539-32-9P 57583-97-8P 57593-72-3P 57607-62-2P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)